

# Cacti with Extremal PI Index

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## Abstract

The vertex PI index  $PI(G) = \sum_{xy \in E(G)} [n_{xy}(x) + n_{xy}(y)]$  is a distance-based molecular structure descriptor, where  $n_{xy}(x)$  denotes the number of vertices which are closer to the vertex  $x$  than to the vertex  $y$  and which has been the considerable research in computational chemistry dating back to Harold Wiener in 1947. A connected graph is a cactus if any two of its cycles have at most one common vertex. In this paper, we completely determine the extremal graphs with the largest and smallest vertex PI indices among all the cacti. As a consequence, we obtain the sharp bounds with corresponding extremal cacti and extend a known result.

**Keywords:** Distance, Extremal bounds,  $PI$  index, Cacti.

**AMS subject classification:** 05C90, 05C12, 05C05

## 1 Introduction

Let  $G$  be a simple connected graph with vertex set  $V(G)$  and edge set  $E(G)$ . For  $x, y \in V(G)$ , the distance  $d(x, y)$  is the number of edges in a shortest path connecting  $x$  and  $y$ . A vertex is a pendant vertex if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendant if one of its vertices is a pendant vertex. An edge  $e \in E(G)$  is a cut edge if the graph deleting  $e$  contains two components.

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A numerical representation that can preserve a structural property of a graph is mathematically defined as a graphic descriptor or a topological index. The Wiener index is the oldest and most thoroughly examined topological index used in chemistry. In 1947, Harold Wiener[25] applied Wiener index to determine physical properties of types of Alkanes known as Paraffins and defined as

$$W(G) = \sum_{\{x,y\} \subset V(G)} d(x,y).$$

Compared to Wiener index, Szeged index was given by Klavžar and Gutman[16] in 1996 as follows:

$$Sz(G) = \sum_{xy \in E(G)} n_{xy}(x)n_{xy}(y),$$

where  $n_{xy}(x)$  is the number of vertices  $w \in V(G)$  such that  $d(x,w) < d(y,w)$ ,  $n_{xy}(y)$  is the number of vertices  $w \in V(G)$  such that  $d(x,w) > d(y,w)$  and  $w \neq x,y$ . Currently, various work relating Wiener index, Sz index and their chemical meaning have been already studied, referred to the surveys [2, 9, 10, 13]. Based on the considerable success of Wiener index and Sz index, Khadikar[17] proposed edge Padmakar-Ivan( $PI_e$ ) index in 2000, which is used in the field of nano-technology, as follows:

$$PI_e(G) = \sum_{e=xy \in E(G)} [n_{ex}(e|G) + n_{ey}(e|G)],$$

where  $n_{ex}(e|G)$  denotes the number of edges which are closer to the vertex  $x$  than to the vertex  $y$ , and  $n_{ey}(e|G)$  denotes the number of edges which are closer to the vertex  $y$  than to the vertex  $x$ , respectively. The detailed applications of  $PI_e$  indices between chemistry and graph theory are investigated in [3]-[7],[17]-[19]. As this definition does not count edges equidistant from both ends of the edge  $e = xy$ , Khalifeh et al.[20] continued to introduce a new PI index of vertex version below:

$$PI(G) = PI_v(G) = \sum_{xy \in E(G)} [n_{xy}(x) + n_{xy}(y)],$$

where  $n_{xy}(x)$  denotes the number of vertices which are closer to the vertex  $x$  than to the vertex  $y$ . In addition, there are nice results regarding vertex PI index in the study of a computational complexity and the intersection between graph theory and chemistry. In [11], Das and Gutman obtained a lower bound on the vertex PI index of a connected graph in terms of numbers of vertices, edges, pendent vertices, and clique number. Hoji et al.[14] provided exact formulas for the vertex PI indices of Kronecker product of a connected graph  $G$  and a complete graph. Ilić and Milosavljević[15] established basic properties of weighted vertex PI index and proved some lower and upper bounds. Pattabiraman and Paulraja[22] presented the expressions for vertex PI indices of the strong product of a graph and the complete multipartite graph.

The synthetic resins[1] of plastic materials is produced by the composition of phenol and benzene with formaldehyde in a base. There are no common edges between independent benzene rings in the diphenyl ether and the biphenyl. The relation of these rings can be used to partially predict the strength of heat resistance and flame retardancy. Based on this property, we explore another type of graphs: A graph is a cactus if it is connected and all of its blocks are either edges or cycles, i.e., any two of its cycles have at most one common vertex. Denote the cacti of  $n$  vertices and  $k$  pendent vertices as  $\mathcal{C}_{n,k}$  with  $n \geq k \geq 0$ . Let  $\lfloor x \rfloor$  be the largest integer which is less than or equal to  $x$ . Up to now, many results were obtained concerning the cacti between chemistry and graph theory. In [21], Li and Yang determined sharp upper and lower bounds of the cacti in  $\mathcal{C}_{n,k}$  for special chemical indices of Zagreb indices. Feng and Yu[12] established the cacti in  $\mathcal{C}_{n,k}$  with the smallest hyper-Wiener indices, which is a renovated version of Wiener index. Wang and Tan[23] characterized the extremal cacti having the largest Wiener and hyper-Wiener indices in  $\mathcal{C}_{n,k}$ . Wang and Kang[24] found the extremal bounds of another chemical index, Harary index, for the cacti  $\mathcal{C}_{n,k}$ . Chen[8] gave the first three smallest Gutman indices among the cacti.

Motivated by the results of chemical indices and their applications, it is worth noting that it may be much interesting to characterize the cacti in  $\mathcal{C}_{n,k}$  with maximum and minimum vertex PI indices. The concept of vertex PI index yields the following fact.

**Fact 1** *Let  $G \in \mathcal{C}_{n,k}$  with  $n \geq k \geq 0$ , then*

- (i) *If  $G$  is  $C_3$ ,  $C_4$  or  $C_5$ , then  $PI(G) = 0, 8, 10$ .*
- (ii) *If  $G$  is  $C_3$  attaching a pendent edge  $e$  (say  $C_3 \cup e$ ), then  $PI(G) = 4$ .*

In this paper, we determine graphs with the largest and smallest vertex PI indices in  $\mathcal{C}_{n,k}$ , and provide the extremal cacti in Figs 1, 2, which extends Das and Gutman's result[11] by excluding the number of edges and cliques for the cacti. Our main results are as follows. (In Figs 1 and 2,  $\circ$  means that the vertex maybe exist.)

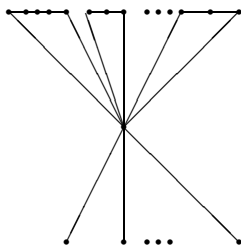
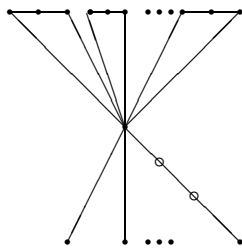


Fig. 1

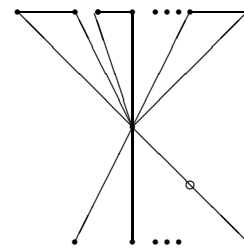


Fig. 2

**Theorem 1** *Let  $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4, C_5\}$  with  $n \geq k \geq 0$ , then  $PI(G) \leq (n - 1 + \lfloor \frac{n-k-1}{3} \rfloor)(n - 2)$ , where the equality holds if and only if  $G$  is a tree for  $n \leq k + 3$  and otherwise, one of the following statements holds (See Fig. 1):*

- (i) All cycles have length 4 and there are at most  $k + 2$  cut edges.
- (ii) All cycles have length 4 except one of length 6 and there are exact  $k$  pendent edges.

**Theorem 2** Let  $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4\}$  with  $n \geq k \geq 0$ , then  $PI(G) \geq (n-1)(n-2) - 2\lfloor \frac{n-k-1}{2} \rfloor$ , where the equality holds if and only if  $G$  is a tree for  $n \leq k+2$  and otherwise, all cycles have length 3 and there are at most  $k+1$  cut edges (See Fig. 2).

## 2 Main proofs

Firstly, we provide some lemmas which are important in the proof of our main results.

**Lemma 1:** Let  $G \in \mathcal{C}_{n,k}$  and  $e \in E(G)$ . Then

- (i)  $PI(e) \leq n - 2$ , the equality holds if  $e$  is a cut edge or an edge of an even cycle.
- (ii) If  $e$  is an edge of an odd cycle  $C_o$ , then  $PI(e) \leq n - 3$ . Furthermore, if  $G = C_o$ , then  $PI(e) = n - 3$ .
- (iii) For each odd cycle  $C$  of  $G$ ,  $PI(C) = (n - 2)(|C| - 1) - 2$ .

**Proof:** Assume that  $e = uv \in E(G)$ . Since  $PI(e)$  counts at most  $n - 2$  vertices, then  $PI(e) \leq n - 2$ . If  $e$  is a cut edge, then  $G - e$  contains two components  $G_1$  and  $G_2$ . Thus, all vertices of  $G_1$  are closer to one of  $\{u, v\}$ , say  $u$ , and all vertices of  $G_2$  are closer to  $v$ . Thus,  $PI(e) = n_e(u) + n_e(v) = n - 2$  if  $e$  is a cut edge. Let  $C = v_1 v_2 \dots v_a v_1$  be a cycle of  $G$  and  $v_l v'_l \in E(C)$ . Since  $G$  is a cactus, then  $G - E(C)$  contains  $a$  components  $B_1, B_2, \dots, B_a$  such that  $v_i \in V(B_i)$ . If  $a$  is even, then  $d(v_l, v_i) \neq d(v'_l, v_i)$  for  $1 \leq i \leq a$ , and  $d(v_l, u_i) \neq d(v'_l, u_i)$  with  $u_i \in V(B_i)$ . We obtain that  $PI(e) = n - 2$  if  $C$  is even. Thus, (i) is true.

For  $C = C_o$ ,  $a$  is odd. Then there exists a unique vertex  $v_t \in V(C)$  such that  $d(v_l, v_t) = d(v'_l, v_t)$ , that is,  $PI(e) \leq n - 3$ . When  $G = C_o$ , we see  $PI(e) = n - 3$ . Thus, (ii) is true.

For (iii),  $a$  is odd and  $\sum_{i=1}^a |B_i| = n$ . Note that if  $d(v_l, v_t) = d(v'_l, v_t)$  with  $v_t \in V(C)$ , then  $d(v_l, u_t) = d(v'_l, u_t)$  with  $u_t \in V(B_t)$ . Similarly, if  $d(v_l, v_t) \neq d(v'_l, v_t)$  with  $v'_t \in V(C)$ , then  $d(v_l, u'_t) \neq d(v'_l, u'_t)$  with  $u'_t \in V(B_t)$ . Thus,  $PI(v_l v'_l) = n - 2 - |B_t|$  with  $t \neq l, l'$ . It induces that

$$\begin{aligned}
 PI(C) &= \sum_{e \in E(C)} PI(e) = \sum_{i=1}^a (n - 2 - |B_i|) \\
 &= a(n - 2) - \sum_{i=1}^a |B_i| \\
 &= |C|(n - 2) - n \\
 &= (|C| - 1)(n - 2) - 2
 \end{aligned}$$

and Lemma 1 is true.  $\square$

**Lemma 2:** Let  $C$  be a cycle of  $G$ . Define *Transformation 1*:  $G_1 = G - xy$  with  $xy \in E(G) - E(C)$  and *Transformation 2*:  $G_2 = G + x'y'$ , where at least one of  $\{x', y'\}$  are in  $V(G) - V(C)$ . If  $G_1, G_2 \in \mathcal{C}_{n,k}$  and  $e \in E(C)$ , then  $PI(e) = PI_{G_1}(e) = PI_{G_2}(e)$ .

**Proof:** Let  $C = v_1 v_2 \dots v_a v_1$ ,  $v_l v'_l \in E(C)$ . Then  $G - E(C)$  contains  $a$  components  $B_1, B_2, \dots, B_a$  such that  $v_i \in V(B_i)$ . Since  $G$  is a cactus, then for  $v_i \in V(C)$ , if  $d(v_l, v_i) = d(v'_l, v_i)$ , we obtain  $d(v_l, u_i) = d(v'_l, u_i)$  with  $u_i \in V(B_i)$ . Similarly, if  $d(v_l, v_i) \neq d(v'_l, v_i)$ , we obtain  $d(v_l, u_i) \neq d(v'_l, u_i)$  with  $u_i \in V(B_i)$ . Note that  $G_1$  and  $G_2$  contain the same cycle  $C$  as  $G$ , and the components  $B_j^i$  of  $G_i - C$  with  $v_j \in V(B_j^i)$  has the property that  $V(B_j^i) = V(B_j^i)$ . Then for  $v_i \in V(C)$ , if  $d(v_l, v_i) = d(v'_l, v_i)$ , then  $d_{G_1}(v_l, v_i) = d_{G_1}(v'_l, v_i)$  and  $d_{G_2}(v_l, v_i) = d_{G_2}(v'_l, v_i)$ ,  $d_{G_1}(v_l, u_i) = d_{G_1}(v'_l, u_i)$  with  $u_i \in V_{G_1}(B_i)$  and  $d_{G_2}(v_l, u_i) = d_{G_2}(v'_l, u_i)$  with  $u_i \in V_{G_2}(B_i)$ . Similarly, if  $d(v_l, v_i) \neq d(v'_l, v_i)$ , then  $d_{G_1}(v_l, v_i) \neq d_{G_1}(v'_l, v_i)$  and  $d_{G_2}(v_l, v_i) \neq d_{G_2}(v'_l, v_i)$ ,  $d_{G_1}(v_l, u_i) \neq d_{G_1}(v'_l, u_i)$  with  $u_i \in V_{G_1}(B_i)$  and  $d_{G_2}(v_l, u_i) \neq d_{G_2}(v'_l, u_i)$  with  $u_i \in V_{G_2}(B_i)$ . Thus,  $PI(e) = PI_{G_1}(e) = PI_{G_2}(e)$  and Lemma 2 is true.  $\square$

**Lemma 3:** If  $G \in \mathcal{C}_{n,k}$  contains  $t_1$  cycles of lengths  $\{l_1, l_2, \dots, l_{t_1}\}$  and  $t_2 \geq k$  cut edges, then  $PI(G)$  is unique and these cycles can be shared a common vertex  $u_0$ ,  $k - 1$  pendent edges can be adjacent to  $u_0$  and a path of length  $t_2 - k + 1$  can be adjacent to  $u_0$ . (See Fig. 2)

**Proof:** By Lemma 1(i) and (iii), PI values with cycles of fixed lengths and fixed number of cut edges are determined. Then  $PI(G) = \sum_C$  is a cycle of  $G$   $\sum_{e \in E(C)} PI(e) + \sum_e$  is an cut edge of  $G$   $PI(e)$  is unique. By recombining these cycles and cut edges,  $t_1$  cycles can have a common vertex  $u_0$ ,  $k - 1$  pendent edges can be adjacent to  $u_0$  and a path of length  $t_2 - k + 1$  can be adjacent to  $u_0$ . Thus, Lemma 3 is true.  $\square$

**Lemma 4:** Let  $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$ , if  $PI(G)$  attains the maximal value, then the length of each cycle, if any, is even.

**Proof:** If  $G$  has a cycle, then  $n \geq 3$ . Assume that there is an odd cycle  $C_{2t+1} = u_1 u_2 \dots u_{2t} u_{2t+1} u_1$  with  $t \geq 1$ . If all vertices of  $C_{2t+1}$  have degree 2, then  $G = C_{2t+1}$ . Since  $G \neq C_3, C_5$ , then  $n \geq 7$ . By Lemma 1(ii),  $PI(e) = n - 3$  for  $e \in E(C_{2t+1})$  and  $PI(C_{2t+1}) = n(n - 3)$ . By Lemma 1(iii),  $PI(G) = (n - 2)(2t) - 2$ . We build a new graph  $G' = (G - \{u_1 u_{2t+1}\}) \cup \{u_1 u_{2t-2}, u_{2t+1} u_{2t-2}\}$ . Then  $G'$  contains a cycle  $C'_1 = u_{2t-2} u_{2t-1} u_{2t} u_{2t+1} u_{2t-2}$  of length 4 and a cycle  $C'_2 = u_1 u_2 \dots u_{2t-2} u_1$  of length  $2t - 2$ . By Lemma 1(i),  $PI(G') = PI(C'_1) + PI(C'_2) = (n - 2)(2t + 2)$ . Thus,  $PI(G') > PI(G)$ , contradicted that  $PI(G)$  is maximal.

Thus, there is a vertex of degree at least 3 in  $C_{2t+1}$ . If the vertex of degree 3 is unique, say  $u_1$ , then there exists a pendent path  $u_1 v_1 v_2 \dots$ . Set  $G_0 = (G - \{u_1 u_2\}) \cup \{u_2 v_1\}$ , then  $G_0 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$ . By Lemma 1, we obtain  $PI(G_1) > PI(G)$ , a contradiction. If at least two vertices of  $\{u_1, u_2, u_3\}$  has degree at least two, say  $u_1, u_2$ . Set  $G_1 = G - \{u_1 u_2\}$ , then  $G_1 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$ . By Lemma 1, we obtain  $PI(G) = PI(C) + k(k + 1) = k(k + 3)$  and  $PI(G_1) = (k + 1)(k + 3) > PI(G)$ , a contradiction. If  $t \geq 2$ , we construct a new graph  $G_2$  such that  $G_2 = G - \{u_1 u_{2t+1}\} \cup \{u_1 u_{2t}\}$  with  $d_G(u_{2t+1}) \geq 3$ . Then  $G_2 \in$

$\mathcal{C}_{n,k}$ ,  $C_{2t}$  is an even cycle and  $u_{2t}u_{2t+1}$  is a cut edge. By Lemma 1 and 2,

$$\begin{aligned} PI(G_2) - PI(G) &= (PI(u_{2t}u_{2t+1}) + PI(C_{2t})) - PI(C_{2t+1}) \\ &= (n-2)(2t+1) - [(n-2)(2t) - 2] \\ &> 0, \end{aligned}$$

contradicted that  $PI(G)$  is maximal. Therefore, each cycle, if any, is even and Lemma 4 is true.  $\square$

**Lemma 5:** Let  $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$  with  $n \geq k+4$ , if  $PI(G)$  attains the maximal value, then all cycles are length 4 except at most one of them is 6.

**Proof:** By Lemma 4, all cycles are even. If there exists a cycle  $C = u_1u_2\dots u_{2t}u_1$  with  $t \geq 4$ . Set  $G_1 = (G - \{u_1u_{2t}\}) \cup \{u_1u_4, u_4u_{2t}\}$ . Then  $G_1 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e\}$  and  $|E(G_1)| = |E(G)| + 1$ . Since each edge of  $G_1$  is either a cut edge or an edge of an even cycle, then  $PI(G_1) > PI(G)$  by Lemma 1(i), that is, the length of cycles are at most 6. Now suppose that there are two cycles of length 6. By Lemma 3, we can assume these two cycles share a common vertex  $u_1$ , say  $C_1 = u_1u_2\dots u_6u_1$  and  $C_2 = u_1v_2\dots v_6u_1$ . Set  $G_2 = G - \{u_1u_2, u_3u_4, u_1v_2\} \cup \{u_1u_4, u_2v_2, u_3v_3, u_1v_3\}$ . Then  $G_2 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e\}$  and  $|E(G_2)| = |E(G)| + 1$ . Since each edge of  $G_2$  is either a cut edge or an edge of an even cycle, then  $PI(G_1) > PI(G)$ , that is, there are at most one cycle of length 6 and Lemma 5 is true.  $\square$

**Lemma 6:** Let  $G \in \mathcal{C}_{n,k} - \{C_4\}$ , if  $PI(G)$  attains the minimal value, then the length of each cycle, if any, is odd.

**Proof:** Suppose  $G$  has an even cycle  $C_{2t} = u_1u_2\dots u_{2t}u_1$ , then  $n \geq k+4$  and  $t \geq 2$ . If all vertices of  $G$  have degree 2, then  $G = C_{2t}$  and  $n = 2t$ . By Lemma 1(i),  $PI(G) = n(n-2) = 2t(2t-2)$ . Since  $G \neq C_4$  and  $t \geq 3$ , set  $G_1 = (G - \{u_1u_2\}) \cup \{u_1u_4, u_2u_4\}$ . Then  $G_1 \in \mathcal{C}_{n,k} - \{C_4\}$ ,  $C_{1,3} = u_2u_3u_4u_2$  is an odd cycle and  $C_{1,2t-2} = u_1u_4u_5\dots u_{2t}u_1$  is an even cycle. By Lemma 1(i) and (iii),  $PI(G_1) = PI(C_{1,3}) + PI(C_{1,2t-2}) = (n-2)2-2 + (n-2)(2t-2) = 2t(2t-2) - 2 < PI(G)$ , contradicted that  $PI(G)$  is minimal. If there exists a vertex  $u_2$  with  $d(u_2) \geq 3$ , then we construct a new graph  $G_2 = (G - \{u_1u_2\}) \cup \{u_1u_3\}$ . Then  $G_2 \in \mathcal{C}_{n,k}$ ,  $u_2u_3$  is a cut edge and  $C' = u_1u_3u_4\dots u_{2t}u_1$  is an odd cycle. By Lemma 1 and 3,

$$\begin{aligned} PI(G_2) - PI(G) &= (PI_{G_2}(u_2u_3) + PI_{G_2}(C')) - PI(C_{2t}) \\ &= [(n-2) + (n-2)(2t-2) - 2] - 2t(n-2) \\ &= -n < 0. \end{aligned}$$

Thus,  $PI(G_2) < PI(G)$ , contradicted that  $PI(G)$  is minimal. Therefore, each cycle, if any, is odd and Lemma 6 is true.  $\square$

**Lemma 7:** Let  $G \in \mathcal{C}_{n,k} - \{C_4\}$  with  $n \geq k+3$ , if  $PI(G)$  attains the minimal value, then all cycles have length 3.

**Proof:** By Lemma 6, we only consider all cycles of  $G$  are odd. Suppose that there is an odd cycle of length greater than 3, say  $C_{2t+1} = u_1u_2\dots u_{2t+1}u_1$  with  $t \geq 2$ . Set a new

graph  $G_1 = (G - \{u_{2t-1}u_{2t}\}) \cup \{u_1u_{2t-1}, u_1u_{2t}\}$ . Then  $G_1 \in \mathcal{C}_{n,k}$  and we will show that  $PI(G_1) < PI(G)$ . Let  $C_1 = u_1u_2...u_{2t-1}u_1$  and  $C_2 = u_1u_{2t}u_{2t+1}u_1$ . By Lemma 1(iii),  $PI(C) = (n-2)(|C|-2) - 2 = 2t(n-2) - 2$  and  $PI(C_1) + PI(C_2) = [(n-2)(|C_1|-2) - 2] + [(n-2)(|C_2|-2) - 2] = 2t(n-2) - 4$ . Thus,  $PI(C_1) + PI(C_2) < PI(C)$ . By Lemma 2,  $PI(G_1) - PI(G) = PI(C_1) + PI(C_2) - PI(C) < 0$  and Lemma 7 is true.  $\square$

Now, we turn to prove the main results of this paper.

**Proof of Theorem 1.** All length of cycles, if any, are even by Lemma 4. Since  $e \in E(G)$  is either a cut edge or an edge of an even cycle, then  $PI(e) = n - 2$  by Lemma 1(i). Thus,  $PI(G) = |E(G)|(n - 2)$  and it needs to maximize  $|E(G)|$ . For  $n \leq k + 3$ ,  $\lfloor \frac{n-k-1}{3} \rfloor = 0$  and  $PI(G) = (n - 1)(n - 2)$ . Thus, Theorem 1 is true. For  $n \geq k + 4$ , all length of cycles are 4 except at most one of them is 6 by Lemma 5. By Lemma 3, all cycles of  $G$  have a common vertex  $u_0$ ,  $k - 1$  pendent edges are adjacent to  $u_0$  and a path of length  $t_2 - k + 1$  is adjacent to  $u_0$ .

Assume that there exist a cycle  $C_6 = u_0u_1u_2u_3u_4u_5u_0$  and  $G$  contains more than  $k + 1$  cut edges, then  $G$  has a path  $u_0v_1v_2...$  of length more than 2. Set  $G_1 = (G - \{u_2u_3\}) \cup \{u_2v_1, u_0u_3\}$ , then  $G_1 \in \mathcal{C}_{n,k}$  and  $|E(G_1)| = |E(G)| + 1$ . Since  $e \in E(G_1)$  is either a cut edge or an edge of an even cycle, then  $PI(e) = n - 2$  and  $PI(G_1) = (n - 2)|E(G_1)| > PI(G) = (n - 2)|E(G)|$ , contradicted that  $PI(G)$  is maximal. Thus,  $G$  contains exact  $k$  pendent edges. Next we will show that if all length of cycles are 4, then  $G$  contains at most  $k + 2$  cut edges. Otherwise, there exist a path  $u_0v_1v_2...$  of length at least 4 by Lemma 3. Set  $G_2 = G \cup \{u_0v_3\}$ , then  $G_2 \in \mathcal{C}_{n,k}$  and  $|E(G_2)| = |E(G)| + 1$ . Since  $e \in E(G_1)$  is either a cut edge or an edge of an even cycle, then  $PI(e) = n - 2$  and  $PI(G_2) = (n - 2)|E(G_2)| > PI(G) = (n - 2)|E(G)|$ , contradicted that  $PI(G)$  is maximal. Note that for  $n \geq k + 4$ , the number of cycles of  $G$  is  $\lfloor \frac{n-k-1}{3} \rfloor$  and the number of edges of  $G$  is  $n - 1 + \lfloor \frac{n-k-1}{3} \rfloor$ . Thus,  $PI(G) = (n - 1 + \lfloor \frac{n-k-1}{3} \rfloor)(n - 2)$  and Theorem 1 is true.  $\square$

**Proof of Theorem 2.** For  $n \leq k + 2$ ,  $\lfloor \frac{n-k-1}{2} \rfloor = 0$  and  $PI(G) = (n - 1)(n - 2)$  by Lemma 1. Thus, Theorem 2 is true. For  $n \geq k + 3$ , the length of each edge of  $G$  is 3 by Lemma 7. Next we will show that  $G$  contains at most  $k + 1$  cut edges. Assume that  $G$  contains at least  $k + 2$  cut edges. By Lemma 3, all cycles of  $G$  have a common vertex  $u_0$ ,  $k - 1$  pendent edges are adjacent to  $u_0$  and a path of length at least  $(k + 2) - k + 1 = 3$  is adjacent to  $u_0$ . Denote the path as  $u_0v_1v_2v_3...$ , set  $G_1 = G \cup \{u_0v_2\}$ . By Lemma 1(iii) and 2,  $PI(G_1) - PI(G) = PI_{G_1}(v_0u_1u_2v_0) - PI(u_0v_1) - PI(v_1v_2) = [(n - 2)(3 - 1) - 2] - (n - 2) - (n - 2) = -2 < 0$ . Thus,  $PI(G_1) < PI(G)$ , contradicted that  $PI(G)$  is minimal. Note that for  $n \geq k + 3$ , the number of cycles of length 3 is  $\lfloor \frac{n-k-1}{2} \rfloor$  and the number of cut edges is  $n - 1 - 2\lfloor \frac{n-k-1}{2} \rfloor$ . Thus,

$$\begin{aligned} PI(G) &= 2(n - 3)(\lfloor \frac{n-k-1}{2} \rfloor) + (n - 1 - 2\lfloor \frac{n-k-1}{2} \rfloor)(n - 2) \\ &= (n - 1)(n - 2) - 2\lfloor \frac{n-k-1}{2} \rfloor, \end{aligned}$$

and Theorem 2 is true.  $\square$

**Remarks.** The maximal and minimal values of vertex PI vertices of cacti are unique, but the cacti achieved the maximal and minimal vertex PI index are not unique. All cacti satisfying the statements in Theorem 1 and Theorem 2 are arrived at the corresponding sharp values. Fig 1 and Fig 2 are special examples achieved the sharp bounds.

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